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EXECUTIVE SUMMARY

5TH INTERNATIONAL CONFERENCE ON FOURIER AND COMPUTERIZED INFRARED SPECTROSCOPY

O. Herrmann and M. Zeya
Analytical Services and Organic Research Sections
Chemical Research Department

The 5th International Conference on Fourier and Computerized Infrared Spectroscopy was held in Ottawa, Ontario from June 24 to June 28, 1985. The conference covered all aspects of infrared spectroscopy from theoretical to industrial applications. Progress in hardware improvements is currently gradual but major software changes appear to be imminent, especially in the area of structure elucidation. The field in general is very software dependent because of the high degree of computerization. This dependency led to some calls for standards and increased "verifiability". An extremely wide range of applications was presented. Many of the applications were based on the high sensitivity and precision of current instrumentation. The conference clearly demonstrated that infrared spectroscopy has been revitalized.

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To: Mr. F.J. Kee
Director of Research

5TH INTERNATIONAL CONFERENCE ON FOURIER AND COMPUTERIZED INFRARED SPECTROSCOPY

O. Herrmann and M. Zeya

The Fifth International Conference on Fourier and Computerized Spectroscopy was held in Ottawa, Ontario from June 24 to June 28, 1985. Twenty invited lectures were presented which provided an overview of the field from theoretical considerations and new developments to industrial applications. In addition, about 210 papers were presented at poster sessions with the authors available for discussions at scheduled times. A book of abstracts may be borrowed from either author.

1.0 INTRODUCTION

The International Conference on Fourier and Computerized Infrared Spectroscopy is held every two years, with the 6th one to be held in Vienna, Austria in 1987. There were about 300 participants, at the current conference, which was fairly good for a conference devoted to a single spectroscopic technique. Although the majority of those attending were, as expected, from Canada and the United States, there were representatives from at least 9 other countries, especially from West Germany, Japan and the United Kingdom. The conference was organized with 4 invited lectures per day and numerous poster sessions with the authors in attendance half a day (odd-numbered papers in the morning and even-numbered papers in the afternoon). This arrangement avoided conflicts among presentations and allowed for much more extensive and personal questioning of the authors. A total of about 210 papers were presented which provided an excellent overview of the state of the art in all aspects of infrared spectroscopy. Highlights of the lecture and papers are presented. In addition to the technical presentations, there was a small (the size was due only to the extreme specialization) instrument exhibit which included every major manufacturer of instruments and several accessory producers.

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2.0 LECTURES AND POSTERS

The lectures provided a good cross-section of the field from theoretical considerations to specific applications. Instead of discussing each lecture and each paper of major interest separately, highlights are grouped below into general topic areas.

2.1 Hardware Developments and Limitations

There have been great improvements in instrumentation in the last decade and some people (manufacturers especially) seemed to be of the opinion that only relatively small refinements remained to be made in the basic instrumentation and that most of the developments would be in software. Current state-of-the-art spectrometers boast resolutions around 0.004 - 0.008 wavenumbers and a spectral range from 190 nm to 4 wavenumbers. A number of excellent lectures and posters pointed out major design flaws in commercial instruments (poorly matched optical pathlengths in double beam instruments, inadequate preamplifiers for detectors and poor quality control were some examples). Correction of these design flaws would lead to significant improvements in performance without any technological advances.

The variety and quality of accessories has continued to increase with special emphasis on surface techniques such as diffuse and specular reflectance, photoacoustic spectroscopy and emission. Sample sizes range from micro (10 micrometer diameter samples using microscope accessories and positioning capability to 2 micrometers; sample layers only Angstroms in thickness) to macro (multi-meter and even kilometer pathlengths - this is, of course, not considering applications in astronomy). However, considerable research is focussed on attempts to extend these limits. Other sampling accessories included automated turntables for handling KBr disks for transmission work or sample cups for diffuse reflectance of powdered samples. A device was also shown which enabled the sampling of flowing powder or pellet streams for near-infrared analysis (eg. moisture content or natural oils in grains). Interfacing of gas chromatographs with infrared spectrometers was also seen as an important area which is still under steady improvement. The use of wide bore capillary columns in these interfaced chromatographs seems to offer the best compromise between good sample separation and adequate sample size for detection. These systems were seen as valuable complements to the now widely accepted gas chromatograph - mass spectrometer systems for the analysis of complex organic mixtures. In contrast, attempts to interface liquid chromatographs with infrared spectrometers have not met with any real success.

2.2 Software Development

Much of the current effort in infrared spectroscopy appears to involve software developments. These developments range from spectrometer control and data conversion (interferogram conversion to spectral data) to pattern recognition and structure elucidation. Some of these developments are discussed below.

2.2.1 Structure Elucidation and Spectral Matching

Structure elucidation or spectral interpretation is definitely a "hot" topic. Instrument manufacturers, major industries and university researchers are all involved in attempts to develop programs which will examine a spectrum and indicate the presence of major structural features. Essentially, these are attempts to develop "expert" systems in infrared spectroscopy and are quite distinct from current spectral matching systems which merely compare the spectra of known compounds in a large library with that of an unknown in hopes of obtaining a match. Because the principles of spectral matching are simpler (but far from trivial), such systems are currently farther advanced in development and are commercially available, although still far from mature. Structure elucidation is "just getting off the ground" and some interesting approaches (quite different from each other) were presented. Until structure elucidation is very far advanced (possibly never that advanced), it will be viewed as a valuable complementary technique to spectral matching rather than a competitive one.

2.2.2 Multicomponent Analysis, Pattern Recognition, Correlation Spectroscopy and Alternate Transform Techniques

Although multicomponent analytical techniques are available which are essentially algorithms for solving simultaneous equations (the analyst picks the wavelengths of interest and the concentration - absorbance relationship of each component must be linear or at least known at each wavelength) such techniques have been combined with pattern recognition methods in near-infrared analysis. The spectra of a set of standards which contain the components of interest in different ratios is examined by the program which then picks the features which best define the mixture. These spectral features may not only be correlated with the component concentrations but also with thermodynamic and physical properties. Interestingly, such pattern-recognition techniques do not seem to have been applied to the more common mid-infrared spectra. Similar pattern recognition techniques have also been applied to unconventional instruments based on rotating filters of polymeric materials with widely different spectra (optimally, the spectra are orthogonal - no features in common). Source "dispersion" occurs only on passing through these filters. The absorbance of a sample is examined with all of the filters in turn and compared with a set of standard materials in order to determine the composition.

Similarly, a single "filter" with varying thickness has been used instead of a filter set. Both of these methods are in early stages of development but offer the possibility of very simple, rugged and cheap instruments for specialized applications. A number of alternatives to Fourier transforms (such as Hadamard transforms) were discussed as offering instumental or mathematical advantages under special conditions.

2.2.3 Software Standards and Testing

A topic of special interest was the need to develop standard methods for testing new software for "bugs" and as a means of proving reliability for legal purposes.

3.0 APPLICATIONS

An extremely broad range of applications was discussed. The applicability of infrared techniques has broadened beyond "mere" identification of materials chiefly because of technical improvements which have made infrared spectroscopy more quantitative in nature, especially in surface analyses. A few examples of applications:

(1) Determination of nerve-gas type components on painted surfaces
(2) Kinetics of epoxy pyrolysis
(3) Pigment analysis of art objects (medieval paintings)
(4) Hydrothermal mineral reactions - related to nuclear repositories
(5) Lubricant and magnetic coating distribution on magnetic disk surfaces

4.0 CONCLUSIONS

Infrared spectroscopy was viewed for some years as a "mature" technique. The advent of commercial Fourier transform instruments has revitalized the field. This conference amply demonstrated that many exciting new developments are underway which will continue to change all aspects of infrared spectroscopy.

Approved by:

O. A. Kupcis
Manager
Chemical Research Dept.

Prepared by:

O. Herrmann
Chemist
Analytical Services Section

M. Zeya
Engineer
Organic Research Section

Reviewed by:

M.R. Booth
Section Head
Analytical Services Section